

CLAIMS

What is claimed is:

1. A composition comprising a quinoxaline derivative having Formula I, shown in Figure 1, wherein:
  - 5         $R^1$  and  $R^2$  are the same or different at each occurrence and are selected from H, F, Cl, Br, alkyl, heteroalkyl, alkenyl, alkynyl, aryl, heteroaryl, alkylenearyl, alkenylaryl, alkynylaryl, alkyleneheteroaryl, alkenylheteroaryl, alkynylheteroaryl,  $C_nH_aF_b$ ,  $OC_nH_aF_b$ ,  $C_6H_cF_d$ , and  $OC_6H_cF_d$ , or both of  $R^5$  together may constitute an arylene or heteroarylene group;
    - 10        a, b, c, and d are 0 or an integer such that  $a+b = 2n + 1$ , and  $c + d = 5$ ,
      - n is an integer, and
      - z is 0 or an integer from 1 through 4.
  - 15        2. The composition of Claim 1, wherein:
    - $R^1$  and  $R^2$  are the same or different at each occurrence and are selected from H, F, Cl, Br, alkyl, heteroalkyl, aryl, heteroaryl, alkylenearyl, alkenylaryl, alkynylaryl, alkyleneheteroaryl, alkenylheteroaryl, alkynylheteroaryl,  $C_nH_aF_b$ ,  $OC_nH_aF_b$ ,  $C_6H_cF_d$ , and  $OC_6H_cF_d$ , or both of  $R^5$  together may constitute an arylene or heteroarylene group, and
      - 20        n is an integer from 1 through 12.
    3. The composition of Claim 1, wherein  $R^1$  is selected from phenylalkenyl, substituted phenylalkenyl, phenylalkynyl, and substituted phenylalkynyl groups.
    - 25        4. The composition of Claim 1, wherein  $R^1$  is selected from alkylacetate and arylcarbonyl groups.
    5. The composition of Claim 1, wherein  $R^1$  is selected from alkyl groups having 1 through 12 carbon atoms.
    6. The composition of Claim 1, wherein  $R^2$  is selected from phenyl groups, substituted phenyl groups, pyridyl groups, and substituted pyridyl groups.
    - 30        7. The composition of Claim 1, wherein both of  $R^2$  together are selected from a biarylene group and a substituted biarylene group.
    8. The composition of Claim 7, wherein  $R^2$  together are selected from a biphenylene, a substituted biphenylene, a bipyridylene, and a substituted bipyridylene.
    - 35        8. The composition of Claim 7, wherein  $R^2$  together are selected from a biphenylene, a substituted biphenylene, a bipyridylene, and a substituted bipyridylene.

9. The composition of Claim 1, wherein the quinoxaline derivative is selected from Formulae I(a) through I(i) and I(k) through I(ag) in Figure 4.

5 10. The composition of Claim 1, wherein the quinoxaline derivative is Formula I(j) in Figure 4.

11. A composition selected having Formula II in Figure 2, wherein:  
R<sup>1</sup> and R<sup>2</sup> are the same or different at each occurrence and are selected from H, F, Cl, Br, alkyl, heteroalkyl, alkenyl, alkynyl, aryl, heteroaryl, alkylenearyl, alkenylaryl, alkynylaryl, alkyleneheteroaryl, alkenylheteroaryl, alkynylheteroaryl, C<sub>n</sub>H<sub>a</sub>F<sub>b</sub>, OC<sub>n</sub>H<sub>a</sub>F<sub>b</sub>, C<sub>6</sub>H<sub>c</sub>F<sub>d</sub>, and OC<sub>6</sub>H<sub>c</sub>F<sub>d</sub>, or both of R<sup>2</sup> together may constitute an arylene or heteroarylene group;  
R<sup>3</sup> is the same or different at each occurrence and is selected from a single bond and a group selected from alkylene, heteroalkylene, arylene, heteroarylene, arylenealkylene, and heteroarylenealkylene;  
Q is selected from a single bond and a multivalent group;  
a, b, c, and d are 0 or an integer such that a+b = 2n + 1, and c + d = 5;

20 m is an integer equal to at least 2;  
n is an integer;  
p is 0 or 1; and  
x is 0 or an integer from 1 through 3.

25 12. The composition of Claim 11, wherein:  
m is an integer from 2 through 10;  
n is an integer from 1 through 12;  
with the proviso that when Q is a single bond, p is 0.

13. The composition of Claim 11, wherein:  
R<sup>1</sup> and R<sup>2</sup> are the same or different at each occurrence and are selected from H, F, Cl, Br, alkyl, heteroalkyl, aryl, heteroaryl, alkylenearyl, alkenylaryl, alkynylaryl, alkyleneheteroaryl, alkenylheteroaryl, alkynylheteroaryl, C<sub>n</sub>H<sub>a</sub>F<sub>b</sub>, OC<sub>n</sub>H<sub>a</sub>F<sub>b</sub>, C<sub>6</sub>H<sub>c</sub>F<sub>d</sub>, and OC<sub>6</sub>H<sub>c</sub>F<sub>d</sub>, or both of R<sup>2</sup> together may constitute an arylene or heteroarylene group;  
35 m is an integer from 2 through 10;  
n is an integer from 1 through 12; and  
p is 0.

14. The composition of Claim 11 wherein Q is selected from a hydrocarbon group with at least two points of attachment, selected from an aliphatic group, a heteroaliphatic group, an aromatic group, and a heteroaromatic group.
- 5        15. The composition of Claim 14 wherein Q is selected from alkylene groups, heteroalkylene groups, alkenylene groups, heteroalkenylene groups, alkynylene groups, and heteroalkynylene groups.
- 10        16. The composition of Claim 11 wherein Q is selected from single-ring aromatic groups, multiple-ring aromatic groups, fused-ring aromatic groups, single-ring heteroaromatic groups, multiple-ring aromatic groups, fused-ring aromatic groups, arylamines, silanes and siloxanes.
17. The composition of Claim 11 wherein Q is selected from Formulae V(a) through V(h) in Figure 5.
- 15        18. The composition of Claim 11, wherein R<sup>1</sup> is selected from phenyl and substituted phenyl groups.
19. The composition of Claim 18, wherein R<sup>1</sup> is selected from substituted phenyl groups having at least one substituent selected from F, Cl, Br, alkyl groups, heteroalkyl groups, alkenyl groups, and alkynyl groups.
- 20        20. The composition of Claim 11, wherein R<sup>1</sup> is selected from alkylacetate and arylcarbonyl groups.
21. The composition of Claim 11, wherein R<sup>1</sup> is selected from alkyl groups having 1 through 12 carbon atoms.
22. The composition of Claim 11, wherein R<sup>2</sup> is selected from phenyl groups, substituted phenyl groups, pyridyl groups, and substituted  
25 pyridyl groups.
23. The composition of Claim 11, wherein R<sup>2</sup> together form a biarylene group.
24. The composition of Claim 23, wherein the biarylene group is selected from biphenylene, substituted biphenylene, bipyridylene, and  
30 substituted bipyridylene.
25. The composition of Claim 11, wherein R<sup>3</sup> is selected from aryl, heteroaryl, alkyl, and heteroalkyl.
26. The composition of Claim 11, wherein R<sup>3</sup> is selected from phenyl and substituted phenyl.
- 35        27. The composition of Claim 11, wherein R<sup>3</sup> is selected from alkyl and heteroalkyl having from 1 through 12 carbon atoms.
28. The composition of Claim 11 selected from Formulae II(b) through II(g) and II(i) through II(k) in Figure 6.

29. The composition of Claim 11 selected from Formulae II(a), II(h), II(l), and II(m).

30. A composition having Formula III in Figure 3, wherein:

- 5         $R^1$  and  $R^2$  are the same or different at each occurrence and are selected from H, F, Cl, Br, alkyl, heteroalkyl, alkenyl, alkynyl, aryl, heteroaryl, alkylenearyl, alkenylaryl, alkynylaryl, alkyleneheteroaryl, alkenylheteroaryl, alkynylheteroaryl,  $C_nH_aF_b$ ,  $OC_nH_aF_b$ ,  $C_6H_cF_d$ , and  $OC_6H_cF_d$ , or both of  $R^5$  together may constitute an arylene or heteroarylene group;
- 10         $R^3$  is the same or different at each occurrence and is selected from a single bond and a group selected from alkylene, heteroalkylene, arylene, heteroarylene, arylenealkylene, and heteroarylenealkylene;
- Q is selected from a single bond and a multivalent group;
- 15        a, b, c, and d are 0 or an integer such that  $a+b = 2n + 1$ , and  $c + d = 5$ ;
- m is an integer equal to at least 2;
- n is an integer2;
- p is 0 or 1; and
- 20        z is 0 or an integer from 1 through 4.

31. The composition of Claim 30 wherein Q is selected from a hydrocarbon group with at least two points of attachment, selected from an aliphatic group, a heteroaliphatic group, an aromatic group, and a heteroaromatic group.

- 25        32. The composition of Claim 31 wherein Q is selected from alkylene groups, heteroalkylene groups, alkenylene groups, heteroalkenylene groups, alkynylene groups, and heteroalkynylene groups.

- 30        33. The composition of Claim 30 wherein Q is selected from single-ring aromatic groups, multiple-ring aromatic groups, fused-ring aromatic groups, single-ring heteroaromatic groups, multiple-ring aromatic groups, fused-ring aromatic groups, arylamines, silanes and siloxanes.

34. The composition of Claim 30 wherein Q is selected from Formulae V(a) through V(h) in Figure 5.

- 35        35. The composition of Claim 30, wherein  $R^1$  is selected from phenylakenyl, substituted phenylalkenyl, and phenylalkynyl, and substituted phenylalkynyl groups.

36. The composition of Claim 30, wherein  $R^1$  is selected from alkylacetate and arylcarbonyl groups.

37. The composition of Claim 30, wherein  $R^1$  is selected from alkyl groups having 1 through 12 carbon atoms.
38. The composition of Claim 30, wherein  $R^2$  is H.
39. The composition of Claim 30, wherein  $R^3$  is selected from aryl, heteroaryl, alkyl, and heteroalkyl.
40. The composition of Claim 30, wherein  $R^3$  is selected from phenyl and substituted phenyl.
41. The composition of Claim 30, wherein  $R^3$  is selected from alkyl and heteroalkyl having from 1 through 12 carbon atoms.
42. An electronic device comprising a photoactive layer and a second layer, wherein at least one layer comprises a quinoxaline derivative having Formula I, shown in Figure 1, wherein:
- $R^1$  and  $R^2$  are the same or different at each occurrence and are selected from H, F, Cl, Br, alkyl, heteroalkyl, alkenyl, alkynyl, aryl, heteroaryl, alkylenearyl, alkenylaryl, alkynylaryl, alkyleneheteroaryl, alkenylheteroaryl, alkynylheteroaryl,  $C_nH_aF_b$ ,  $OC_nH_aF_b$ ,  $C_6H_cF_d$ , and  $OC_6H_cF_d$ , or both of  $R^5$  together may constitute an arylene or heteroarylene group;
- a, b, c, and d are 0 or an integer such that  $a+b = 2n + 1$ , and  $c + d = 5$ ,
- n is an, and
- z is 0 or an integer from 1 through 4.
43. The device of Claim 42, wherein the second layer comprises a quinoxaline derivative having Formula I, shown in Figure 1, and further wherein:
- $R^1$  and  $R^2$  are the same or different at each occurrence and are selected from H, F, Cl, Br, alkyl, heteroalkyl, aryl, heteroaryl, alkylenearyl, alkenylaryl, alkynylaryl, alkyleneheteroaryl, alkenylheteroaryl, alkynylheteroaryl,  $C_nH_aF_b$ ,  $OC_nH_aF_b$ ,  $C_6H_cF_d$ , and  $OC_6H_cF_d$ , or both of  $R^5$  together may constitute an arylene or heteroarylene group, and n is an integer from 1 through 12.
44. The device of Claim 42, wherein  $R^1$  is selected from phenylalkenyl, substituted phenylalkenyl, phenylalkynyl, and substituted phenylalkynyl groups.
45. The device of Claim 42, wherein  $R^1$  is selected from alkylacetate and arylcarbonyl groups.
46. The device of Claim 42, wherein  $R^1$  is selected from alkyl groups having 1 through 12 carbon atoms.

47. The device of Claim 42, wherein  $R^2$  is selected from phenyl groups, substituted phenyl groups, pyridyl groups, and substituted pyridyl groups.

48. The device of Claim 42, wherein both of  $R^2$  together are  
5 selected from a biarylene group and a substituted biarylene group.

49. The device of Claim 42, wherein  $R^2$  together are selected from a biphenylene, a substituted biphenylene, a bipyridylene, and a substituted bipyridylene.

50. The device of Claim 42, wherein the quinoxaline derivative is  
10 selected from Formulae I(a) through I(i) and I(k) through I(ag) in Figure 4.

51. The device of Claim 42, wherein the quinoxaline derivative has Formula I(j) in Figure 4.

52. An electronic device comprising a photoactive layer and a second layer, wherein at least one layer comprises a quinoxaline  
15 derivative selected from Formula II in Figure 2 and Formula III in Figure 3, wherein:

$R^1$  and  $R^2$  are the same or different at each occurrence and are selected from H, F, Cl, Br, alkyl, heteroalkyl, alkenyl, alkynyl, aryl, heteroaryl, alkylenearyl, alkenylaryl, alkynylaryl,  
20 alkyleneheteroaryl, alkenylheteroaryl, alkynylheteroaryl,  $C_nH_aF_b$ ,  $OC_nH_aF_b$ ,  $C_6H_cF_d$ , and  $OC_6H_cF_d$ , or both of  $R^2$  together may constitute an arylene or heteroarylene group;

$R^3$  is the same or different at each occurrence and is selected from a single bond and a group selected from alkylene,  
25 heteroalkylene, arylene, heteroarylene, arylenealkylene, and heteroarylenealkylene;

Q is selected from a single bond and a multivalent group;

a, b, c, and d are 0 or an integer such that  $a+b = 2n + 1$ , and  $c + d = 5$ ;

30 m is an integer equal to at least 2;

n is an integer;

p is 0 or 1; and

x is 0 or an integer from 1 through 3.

53. The device of Claim 52, wherein the second layer comprises a  
35 quinoxaline derivative having Formula II in Figure 2, and further wherein:

m is an integer from 2 through 10;

n is an integer from 1 through 12;

with the proviso that when Q is a single bond, p is 0.

54. The device of Claim 52, wherein the second layer comprises a quinoxaline derivative having Formula II in Figure 2, and further wherein:  
R<sup>1</sup> and R<sup>2</sup> are the same or different at each occurrence and are selected from H, F, Cl, Br, alkyl, heteroalkyl, aryl, heteroaryl, alkylenearyl, alkenylaryl, alkynylaryl, alkyleneheteroaryl, alkenylheteroaryl, alkynylheteroaryl, C<sub>n</sub>H<sub>a</sub>F<sub>b</sub>, OC<sub>n</sub>H<sub>a</sub>F<sub>b</sub>, C<sub>6</sub>H<sub>c</sub>F<sub>d</sub>, and OC<sub>6</sub>H<sub>c</sub>F<sub>d</sub>, or both of R<sup>2</sup> together may constitute an arylene or heteroarylene group;  
m is an integer from 2 through 10;  
n is an integer from 1 through 12; and  
p is 0.
55. The device of Claim 52 wherein Q is selected from a hydrocarbon group with at least two points of attachment, selected from an aliphatic group, a heteroaliphatic group, an aromatic group, and a heteroaromatic group.
56. The device of Claim 52 wherein Q is selected from alkylene groups, heteroalkylene groups, alkenylene groups, heteroalkenylene groups, alkynylene groups, and heteroalkynylene groups.
57. The device of Claim 52 wherein Q is selected from single-ring aromatic groups, multiple-ring aromatic groups, fused-ring aromatic groups, single-ring heteroaromatic groups, multiple-ring aromatic groups, fused-ring aromatic groups, arylamines, silanes and siloxanes.
58. The device of Claim 52, wherein Q is selected from Formulae V(a) through V(h) in Figure 5.
59. The device of Claim 52, wherein the quinoxaline derivative is selected from Formulae II(b) through II(g) and II(i) through II(k) in Figure 6.
60. The device of Claim 52, wherein the quinoxaline derivative is selected from Formulae II(a), II(h), II(l) and II(m).
61. An electronic device of claims 41-59, wherein the device is a light-emitting diode, light-emitting electrochemical cell, or a photodetector.